## CONTENTS

*Special Issue:* Advances in valence bond theory


*Preface* ..... ix

On the historical development of the valence bond method and the non-orthogonality problem
P.O. Löwdin (Gainesville, FL, USA) ..... 1

On the enumeration of basis functions for a double chain of $S = 1/2$ ions: a resonating valence bond problem
K. De Boer, J.J.C. Mulder and W.J.A. Maaskant (Leiden, The Netherlands) ..... 15

On the nature of the oxygen double bond
R. McWeeny (Pisa, Italy) ..... 29

Aspects of hypercoordination and one-electron delocalizations via increased-valence structures
R.D. Harcourt (Parkville, Vic., Australia) ..... 39

Quantum-mechanical and computational aspects of the conjugated-circuit model
N. Trinajstić and S. Nikolić (Zagreb, Yugoslavia) and D.J. Klein (Galveston, TX, USA) ..... 63

A generalized method for the superposition of resonance structures
J.R. Collins and G.A. Gallup (Lincoln, NE, USA) ..... 91

Ab initio valence bond cluster expansion for an alternating infinite chain of hydrogen atoms
R.D. Poshusta (Pullman, WA, USA) and D.J. Klein (Galveston, TX, USA) ..... 103

On the evaluation of non-orthogonal matrix elements
J. Verbeek and J.H. Van Lenthe (Utrecht, The Netherlands) ..... 115

Fully benzenoid systems revisited
M. Randić (Des Moines, IA, USA) ..... 139

On the bonding in $B_2H_6$ and the lone pairs in $H_2O$: the use of localized molecular orbitals in spin-coupled calculations
D.L. Cooper (Liverpool, UK), J. Gerratt (Bristol, UK) and M. Raimondi (Milan, Italy) ..... 155

Covalent, ionic and resonating single bonds
G. Sini, P. Maitre and P.C. Hiberty (Orsay, France) and S.S. Shaik (Beer Sheva, Israel) ..... 163

Hybrids and bond formation: excursions in momentum space
D.L. Cooper and S.D. Loades (Liverpool, UK) and N.L. Allan (Bristol, UK) ..... 189

Has the benzene molecule an extra stability?
R. Janoschek (Graz, Austria) ..... 197

The art of "arrow pushing": is the hyperconjugation model theoretically justified?
N.D. Epiotis (Seattle, WA, USA) ..... 205

The transferability of effective exchange integrals in the non-empirical effective valence bond hamiltonian: a minimal basis study of $H_n$ systems
P. Blaise, P. Breysse and O. Henri-Rousseau (Perpignan, France), J.P. Malrieu and D. Maynau (Toulouse, France) ..... 219

Valence bond approach to the Pariser–Parr–Pople hamiltonian and its application to simple $\pi$-electron systems
X. Li and J. Paldus (Waterloo, Ont., Canada) ..... 249

The ab initio spin-coupled description of the process HCN→CH+N
M. Sironi and M. Raimondi (Milan, Italy), D.L. Cooper (Liverpool, UK) and J. Gerratt (Bristol, UK) ..... 279

*Author Index* ..... 291

*Subject Index* ..... 293